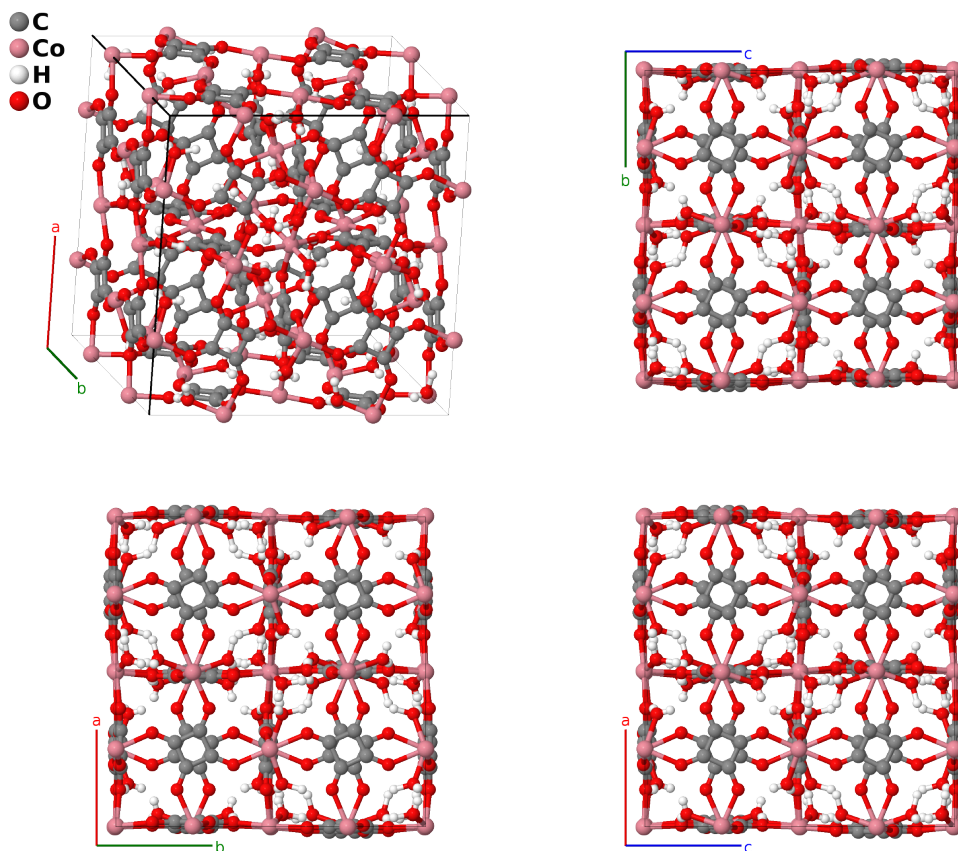


# Co(H<sub>2</sub>O)<sub>2</sub>(C<sub>4</sub>O<sub>4</sub>) Structure: A4BC4D6\_cP360\_222\_2i\_h\_2i\_3i-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/7XG8>

[https://aflow.org/p/A4BC4D6\\_cP360\\_222\\_2i\\_h\\_2i\\_3i-001](https://aflow.org/p/A4BC4D6_cP360_222_2i_h_2i_3i-001)



Prototype	C <sub>4</sub> CoH <sub>4</sub> O <sub>6</sub>
AFLOW prototype label	A4BC4D6_cP360_222_2i_h_2i_3i-001
ICSD	110022
CCDC	187771
Pearson symbol	cP360
Space group number	222
Space group symbol	$Pn\bar{3}n$
AFLOW prototype command	<code>aflow --proto=A4BC4D6_cP360_222_2i_h_2i_3i-001 --params=a, y1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8</code>

**Other compounds with this structure**  
Zn(H<sub>2</sub>O)<sub>2</sub>(C<sub>4</sub>O<sub>4</sub>)

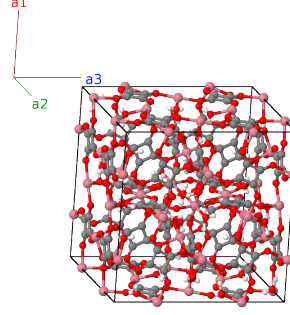
- There is no ICSD entry for (Neeraj, 2002). The ICSD entry is from (Naether, 2002).

### Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + y_1 \mathbf{a}_2 + y_1 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + ay_1 \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_2$	$= \frac{1}{4} \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + y_1 \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - a (y_1 - \frac{1}{2}) \hat{\mathbf{y}} + ay_1 \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_3$	$= \frac{1}{4} \mathbf{a}_1 + y_1 \mathbf{a}_2 - (y_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} - a (y_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_4$	$= \frac{1}{4} \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 - (y_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{4} a \hat{\mathbf{x}} - a (y_1 - \frac{1}{2}) \hat{\mathbf{y}} - a (y_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_5$	$= y_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + y_1 \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + ay_1 \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_6$	$= y_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (y_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - a (y_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_7$	$= -(y_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + y_1 \mathbf{a}_3$	$=$	$-a (y_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} + ay_1 \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_8$	$= -(y_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (y_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a (y_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4} a \hat{\mathbf{y}} - a (y_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_9$	$= y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{10}$	$= -(y_1 - \frac{1}{2}) \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a (y_1 - \frac{1}{2}) \hat{\mathbf{x}} + ay_1 \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{11}$	$= y_1 \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$ay_1 \hat{\mathbf{x}} - a (y_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{12}$	$= -(y_1 - \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$-a (y_1 - \frac{1}{2}) \hat{\mathbf{x}} - a (y_1 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{4} a \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{13}$	$= \frac{3}{4} \mathbf{a}_1 - y_1 \mathbf{a}_2 - y_1 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} - ay_1 \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{14}$	$= \frac{3}{4} \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - y_1 \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + a (y_1 + \frac{1}{2}) \hat{\mathbf{y}} - ay_1 \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{15}$	$= \frac{3}{4} \mathbf{a}_1 - y_1 \mathbf{a}_2 + (y_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + a (y_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{16}$	$= \frac{3}{4} \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + (y_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{3}{4} a \hat{\mathbf{x}} + a (y_1 + \frac{1}{2}) \hat{\mathbf{y}} + a (y_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{17}$	$= -y_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - y_1 \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - ay_1 \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{18}$	$= -y_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (y_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + a (y_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{19}$	$= (y_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - y_1 \mathbf{a}_3$	$=$	$a (y_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} - ay_1 \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{20}$	$= (y_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (y_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a (y_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4} a \hat{\mathbf{y}} + a (y_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{21}$	$= -y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{22}$	$= (y_1 + \frac{1}{2}) \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a (y_1 + \frac{1}{2}) \hat{\mathbf{x}} - ay_1 \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{23}$	$= -y_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-ay_1 \hat{\mathbf{x}} + a (y_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{24}$	$= (y_1 + \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$a (y_1 + \frac{1}{2}) \hat{\mathbf{x}} + a (y_1 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{3}{4} a \hat{\mathbf{z}}$	(24h)	Co I
$\mathbf{B}_{25}$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}}$	(48i)	C I























$$\begin{aligned}
\mathbf{B}_{358} &= -z_8 \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 - x_8 \mathbf{a}_3 &= -az_8 \hat{\mathbf{x}} + a \left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}} & (48i) & \quad \text{O III} \\
\mathbf{B}_{359} &= \left(z_8 + \frac{1}{2}\right) \mathbf{a}_1 - y_8 \mathbf{a}_2 - x_8 \mathbf{a}_3 &= a \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - ay_8 \hat{\mathbf{y}} - ax_8 \hat{\mathbf{z}} & (48i) & \quad \text{O III} \\
\mathbf{B}_{360} &= \left(z_8 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 + &= a \left(z_8 + \frac{1}{2}\right) \hat{\mathbf{x}} + a \left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + a \left(x_8 + \frac{1}{2}\right) \hat{\mathbf{z}} & (48i) & \quad \text{O III} \\
&\quad \left(x_8 + \frac{1}{2}\right) \mathbf{a}_3
\end{aligned}$$

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